

Claims

- SUB 2**
1. Method for information storage and data processing comprising the step of thermo inducing or photo inducing double-bond shifts (DBS) in substituted [4n]-annulenes, thus generating transitions between two different conjugation states with at least one substituent.
2. Method according to claim 1, whereby the two different conjugation states are the conjugation on-state and conjugation off-state of the annulene core  $\pi$ -electrons relative to the substituent  $\pi$ -electrons.
3. Method according to claim 1 ~~or 2~~, whereby said [4n]-annulenes are bicyclic [4n]-annulenes.
4. Method according to claim 3, whereby said bicyclic [4n]-annulenes are heptalenes.
- ~~5. Method according to any of the claims 1 to 4, whereby the [4n]-annulenes which are substituted by at least one group comprising an extended conjugated  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the [4n]-annulene core.~~
- <sup>5</sup>  
6. Method according to claim <sup>4</sup>~~5~~, whereby the [4n]-annulenes are substituted in 1,2- or 1,4-position relative to each other by two groups having an extended and conjugated  $\pi$ -electron system.
- <sup>6</sup>  
7. Method according to <sup>claim 1</sup>~~any of the preceding claims~~, whereby a multitude of [4n]-annulene molecules are arranged in a 1-dimensional or in a 2-dimensional, or in a 3-dimensional way and wherein said conjugation states are spatially non-uniformly modulated.

7  
8. Method according to claim <sup>6</sup>7, whereby a conformationally restricted matrix system is generated by modulating said conjugation states.

8  
9. Method according to <sup>claim 1</sup>any of the preceeding claims, whereby the [4n]-annulene molecules are embedded in a matrix.

9  
10. Method according to claim <sup>8</sup>9, wherein the matrix comprises a low-melting glass or polycarbonates, polyacetates, methacrylates, styrenes and copolymers thereof, as well as copolymers with polymerisable [4n]-annulenes.

10  
11. Method according to any of the claims <sup>6</sup>7-10, whereby a holographic grating is generated by modulating said conjugation states.

11  
12. Method according to ~~one of the claims~~ <sup>6</sup>7-11, wherein the spacially non-uniformly modulated conjugation states are generated by a low-energy laser that provides for a local heating so bring the [4n]-annulenes into switching condition and whereby the laser light causes locally, if required, the switch from the conjugative on-state to the conjugative off-state.

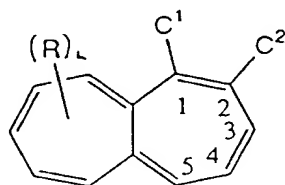
12  
13. Method according to ~~any of the claims~~ <sup>5</sup>7-12, comprising further to said step of modulating a multitude of [4n]-annulene molecules in a 1-dimensional or 2-dimensional or 3-dimensional way and wherein said conjugation states are spacially non-uniformly modulated, a further step wherein at least one of the optical, electrical or magnetic properties being attributable to said switchable conjugation states is determined and processed.

<sup>13</sup>  
14. Method according to ~~any of the preceeding~~ <sup>claim 1</sup> ~~claims~~, wherein said conjugation states are determined by an optical read-out step.

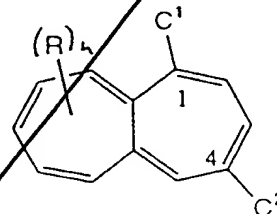
<sup>14</sup>  
15. Method according to ~~any of the preceeding~~ <sup>claim 1</sup> ~~claims~~, wherein the determination of the spacially non-uniformly modulated conjugation states is used for the optical reading of information.

<sup>15</sup>  
16. Method according to ~~any of the preceeding~~ <sup>claim 1</sup> ~~claims~~, wherein the determination of the spacially non-uniformly modulated conjugation states is used for optical switching and computing.

<sup>16</sup>  
SUB B2 17. Substituted [4n]-heptalenes of the general formula (I) or (II) being optically and/or thermally switchable, based on thermal or photochemical double-bond shifts (DBS),



(I)



(II)

whereby  $C^1$  and  $C^2$  represent independently from each other a hydrogen atom, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkoxy group, a substituted or unsubstituted aryl- $C_1$ - $C_{12}$ -alkyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkenyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -conjugated alkenyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkinyl group, a substituted or an unsubstituted phenyl group, a substituted or an unsubstituted heterocyclic group, a cyano group, a nitro group, a thiocyanate group, a  $C_1$ - $C_{12}$ -ester group being optionally polymerisable with copolymers, with the proviso that at least one of

said substituents C<sup>1</sup> and C<sup>2</sup> contains a  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the heptalene core, and

whereby said [4n]-heptalenes can comprise at least one further substituent R being selected from the above indicated groups with n being 0-8,

provided that if one of the at least one further substituents R is a isopropyl group at the position 9 of the heptalene ring, the substituent at the position 6 must not be a methyl group, and

with the proviso that heptalenes having the the following substituents <sup>including their valence isomers</sup> are excluded:

the positions 1 and 2 <sup>or 2</sup> are substituted by a methylester group, <sup>whereby R is H</sup>

the positions 1 and 2 <sup>or 3</sup> are substituted by a methylester group <sup>or position 3 could be substituted by deuterium</sup> and the positions 5, 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 <sup>or 3</sup> are substituted by a methylester group and the positions 4, 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 <sup>or 3</sup> are substituted by a methylester group and the positions 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group and the positions 5, 6 and 10 are substituted by a methyl group,

the positions 1 and 2 <sup>or 3</sup> are substituted by a methylester group and the position 10 is substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group, the position 5 is substituted by a styrene group, the position 7 is substituted by a isopropyl group and the position 10 is substituted by a methyl group, < 1 >

the positions 1 and 2 are substituted by a methylester group, the position 4 is substituted by a

< 1 > = the position 1 is substituted by a methylester group, the positions 2 and 5 are substituted by a  $-\text{CH}=\text{CH}-\text{CH}=\text{CH}-\text{C}_6\text{H}_5$  group, position 7 is an isopropyl- and position 10 a methyl group,

styrene group and the positions 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group, the position 5 is substituted by a  
5 styrene group or a 4-chloro styrene group or a 4-methoxy styrene group, and the positions 6, 8 and 10 are substituted by a methyl group,

the positions 1 and 2 are substituted by a methylester group, the position 5 is substituted by a  
10 methyl group, the position 7 is substituted by an isopropyl group and the position 10 is substituted by a 4-methoxy styrene group or a styrene group,

the positions 1 and 2 are substituted by a methylester group, the positions 5, 6 and 10 are substituted  
15 by a methyl group and the position 8 is substituted by an isobutyl group,

the positions 1 and 2 are substituted by a methylester group, the positions 5 and 10 are substituted  
20 by a methyl group and the position 7 is substituted by an isopropyl group,

the position 1 is substituted by a methyl-  
ester group, the position 2 is substituted by a carboxylic acid group or vice versa, and the positions 5, 6, 8  
and 10 are substituted by a methyl group,

the position 1 is substituted by a methyl-  
25 ester group, the position 2 is substituted by a carboxylic acid group or vice versa, the positions 5 and 10 are substituted by a methyl group and the position 7 is substituted by an isobutyl group,

the positions 1 and 3 are substituted by a  
30 methyl ester group, the position 7 is substituted by an isopropyl group and the positions <sup>8 and 9</sup> 10 <sup>a.c</sup> is substituted by a methyl group,

the position 1 is substituted by a methyl  
35 ester group, the position 2 is substituted by a  $\text{CH}_3\text{-(CH}_2\text{)}_2\text{-C}_6\text{H}_{10}\text{-(CH}_2\text{)-C}_6\text{H}_{10}\text{-COO-}$  group and the positions 5, 6, 8 and 10 are substituted by a methyl group.

~~said substituents C<sup>1</sup> and C<sup>2</sup> contains a  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the heptalene core, and~~

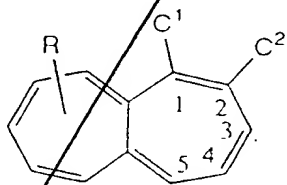
whereby said [4n]-heptalenes can comprise at least one further substituent R being selected from the above indicated groups with n being 0-8,

provided that if one of the at least one further substituents R is a isopropyl group at the position 9 of the heptalene ring, the substituent at the position 5 must not be a methyl group

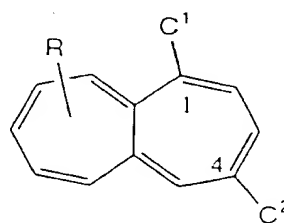
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- 17 18. [4n]-heptalenes according to claim 16, whereby, C<sup>1</sup> and C<sup>2</sup> represent independently from each other a hydrogen atom, a methyl group, a phenyl group, an ethyl ester group, a methyl ester group, a (E)-PhCH=CH group, a (E)-4-MeOC<sub>6</sub>H<sub>4</sub>CH=CH group, a (E)-4-ClC<sub>6</sub>H<sub>4</sub>CH=CH group, a 4-MeOC<sub>6</sub>H<sub>4</sub> group, a -CH=CH-CH=CH-C<sub>6</sub>H<sub>5</sub> group, a -CH=CH-C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4 group, a -CH=CH-C<sub>6</sub>H<sub>4</sub>OMe-4 group, with the proviso that a heptalene being substituted by a methyl ester group at the position 1, a -CH=CH-CH=CH-C<sub>6</sub>H<sub>5</sub> group at the positions 2 and 5, an isopropyl group at the position 7 and a methyl group at the position 9 is excluded.
- 18 19. [4n]-heptalenes according to claim 17, whereby said further substituents R are selected from the group comprising substituted or unsubstituted C<sub>1</sub>-C<sub>10</sub>-alkyl groups or photoactive diazo-containing groups, like azobenzen.

19 20. Method for the preparation of substituted heptalenes of the formula (I) or (II), according to any one of the claims



(I)



(II)

whereby C<sup>1</sup>, C<sup>2</sup>, R and n are as above defined, comprising the steps of

(a) obtaining a heptalene-dicarboxylate by a reaction of a correspondingly substituted azulene with acetylenedicarboxylate, ~~and optionally~~

~~(b) transforming said methyl substituent at the position 1 of the heptalene ring into the desired conjugated substituent having an extended  $\pi$ -electron system.~~

<sup>20</sup> 21. Method according to claim <sup>19</sup> 20, whereby a heptalene-4,5-dicarboxylate carrying a methyl substituent at the position 1 of the heptalene ring is obtained.

<sup>21</sup> 22. Method according to claim <sup>19</sup> 20 or <sup>20</sup> 21, further comprising a step (c) wherein at least one of the carboxylate groups within the heptalene ring is replaced by a conjugated substituent containing an extended  $\pi$ -electron system.

<sup>22</sup> 23. Method according to claim <sup>21</sup> 22, wherein the carboxylate group at the position 4 of the heptalene ring is replaced by a conjugated substituent containing an extended  $\pi$ -electron system.

<sup>23</sup> 24. An optical storage device comprising at least one substituted  $[4n]$ -annulene according to ~~one of the claims 17-19.~~

<sup>24</sup> 25. A non-linear optical device comprising at least one substituted  $[4n]$ -annulene according to ~~to one of the claims 17-19.~~

<sup>25</sup> 26. Use of substituted  $[4n]$ -annulenes <sup><1></sup> undergoing thermally induced or photo-induced double-bond shifts (DBS) thus generating two different conjugation states with at least one substituent, for information storage and data processing.

< 1 > = which are substituted by at least one group comprising an extended conjugated  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the  $[4n]$ -annulene core

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